Ethyl hydrogen glutarate

1070-62-8 | DTXSID20147865

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.06e-01

Global applicability domain: Inside

Local applicability domain index: 5.75e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

Image not found
2,5-Hexanedione
Measured: -0.270
Predicted: 6.68e-02

Image not found
Propanedioic acid, dimethyl-
Measured: 0.39
Predicted: 2.43e-01

Image not found
Methyl levulinate
Measured: -0.130
Predicted: 1.46e-01

Image not found
Ethyl acetoacetate
Measured: 0.25
Predicted: 2.07e-01